UNIVERSITÀ DEGLI STUDI DI MILANO

SEMINARI ERC

ERC GRANT SEMICOMPLEX

Data ***Giovedì 19 Gennaio 2017, ore 14:30***
Aula Bianchi, Dipartimento di Chimica

Oratore **Dr. Huaqing Li, Università delgi Studi di Milano**

Titolo**:** **Keep Dynamical Quantum Effect in Multi-dimensional MD**

Coordinatore **Prof. Michele Ceotto,** *Dipartimento di Chimica*

As we approach to the quantum world, there are a lot of fancy properties that we can not mimic from a classical perspective. Such as tunneling, etc. However, for computational chemists or physicists, one is assumed to take a lot of effort to achieve these quantum effects for multi-dimensional systems. On the other hand, the classical MD scales nicely with dimensionality and runs trajectories independently of each other. Thus, it will be an ambitious goal for scientists to bridge the quantum world with a classical-like simulation using independent trajectories. Such attempt is repaid by its better results in applications and philosophical interpretations.

We adopt an effective quantum force to describe the dynamics in Wigner space. This is based on the method of Linearized Semi-Classical Initial Value Representation(LSCIVR) which propagate the trajectories independently and Entangled Trajectories Molecular Dynamics(ETMD) which accounts for the effect of the nearby trajectories as entanglement. And we try to propagate each trajectory independently without omitting the dynamical quantum effect. Our method is able to approximately describe the exact equation of motion of the Wigner function, which is the Wigner Liouville equation. The results are as accurate but numerical cost is reduced compared to the ETMD method.

In this seminar, I will summarize the application of the quantum force we derived to apply on a series of applications from reaction, diffusion to IR spectroscopy. There one will be interested to find out that the quantum effect can be carried out by trajectories and produces decent results compared with full-quantum results in different applications. Also the dynamics we implement is able to be applied to much higher dimensional applications in biology and material science, etc.